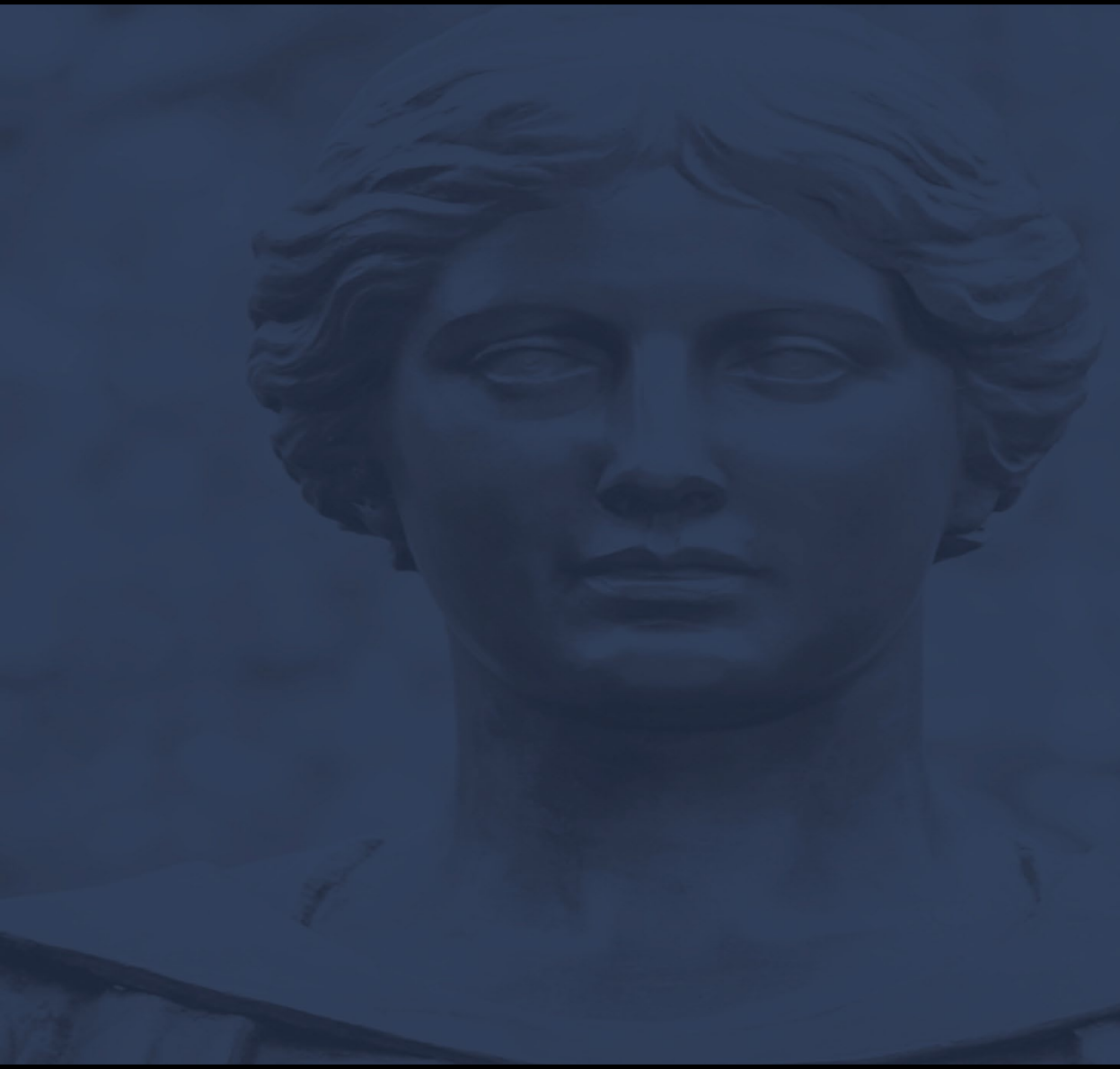
ILLINOIS



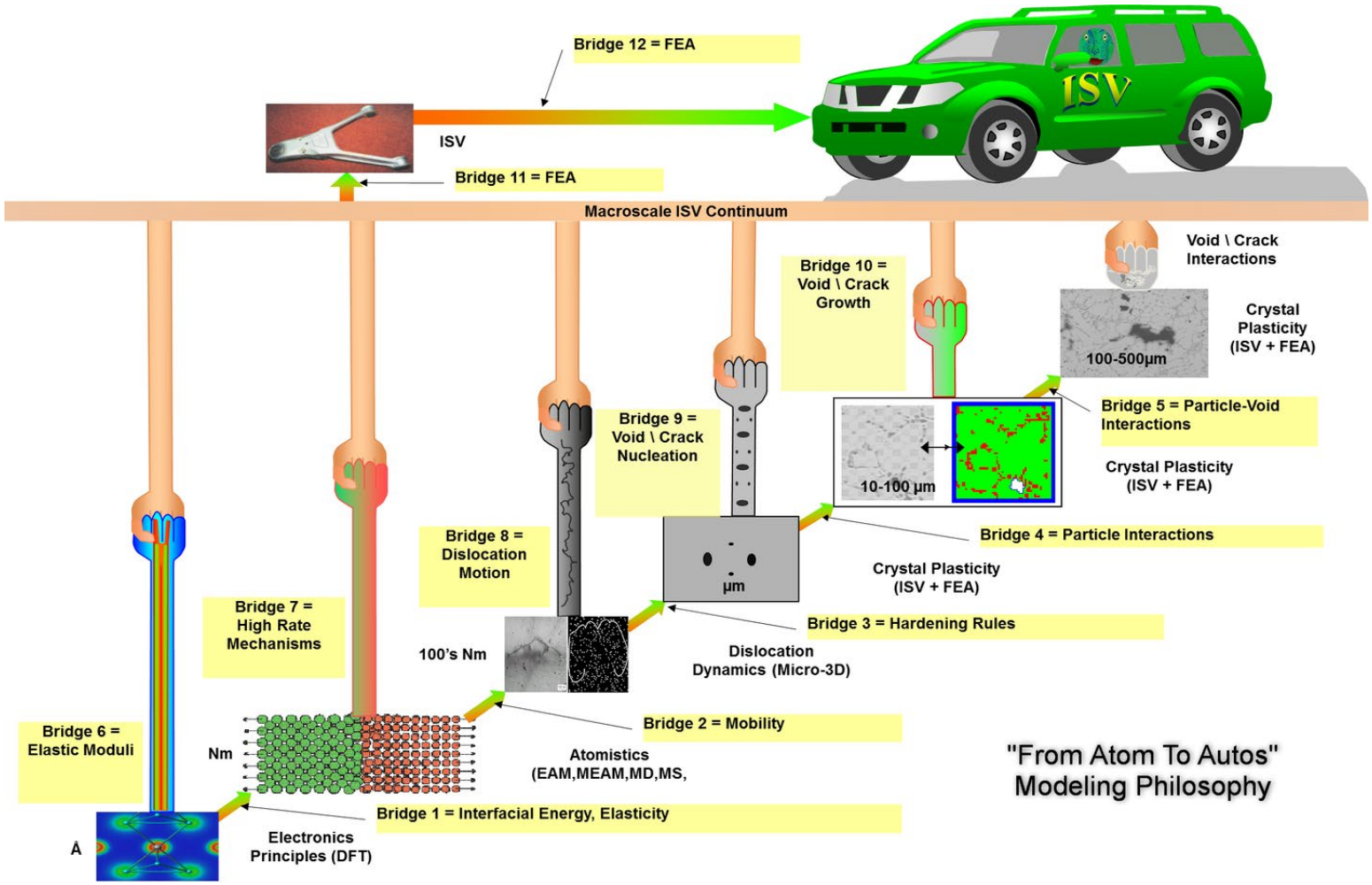
Machine Learning in Material Design

Dr. Yumeng Li

Office: TB 212

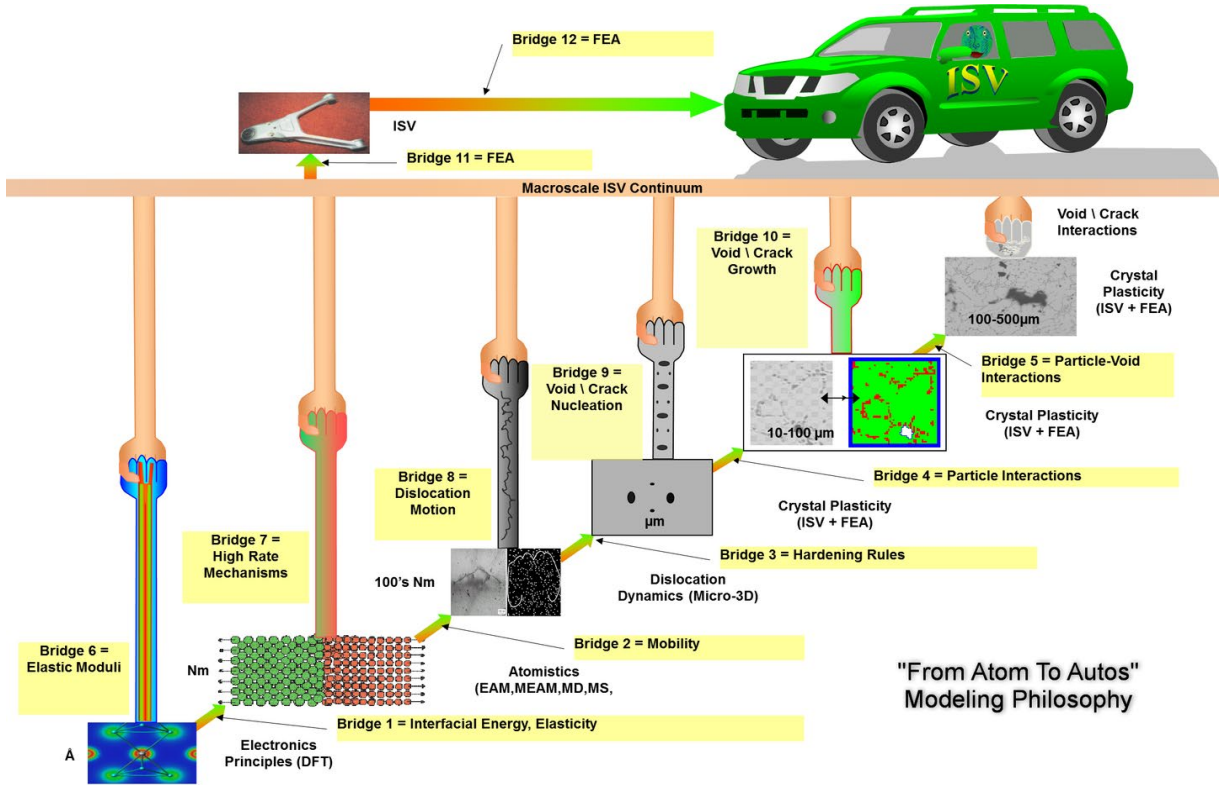
Email: Yumengl@illinois.edu

ICME-Computational simulations



Computational simulations

- First principal calculations
  - Electron structure
- Atomistic simulations
  - Atomic structure
- Micromechanics simulations
  - Microstructure
- Macroscale simulations
  - Material
  - Structure
  - Boundary conditions
  - Environmental conditions



First principal calculations

- First principle calculations determine the electronic properties of an assemble of atoms using the laws of quantum mechanics
  - Schrödinger equation: a partial differential equation for wave function
  - Density functional theory: instead of solving many-body Schrödinger equation for all electrons, the concept of electron density is used to reformulate the problem.

- Popular DFT software: VASP, Quantum ESPRESSO, and Gaussian

- From first principal calculations, the following can be obtained
  - Total energy of the system
  - Optimized atomic structure
  - Band structures
  - Charge densities

Atomistic Simulations

- Atomistic simulations consist three principal steps:
  1. Construction of the model for the target material system
     - Atom type
     - Placement
     - Bonding

  2. Calculation of atomistic trajectories
  3. Analysis of trajectories to obtain properties, i.e., E, T, p, etc.

- Monte Carlo simulations vs Molecular Dynamics simulations

Monte Carlo Simulations

- Monte Carlo simulations generate positions and momenta by stochastic methods, such that the atomic configurations depends only on the previous configuration.

- When the outcome of a random event in a sequence depends only on the outcome of the immediately previous event, the sequence is classified as Markov chain

- In Monte Carlo simulations, a fixed number of atoms are simulated in a fixed V at some temperature T following the general steps below:
  - Initialize at some state and determine the energy
  - Propose a new state from a proposal distribution
  - Accept or reject the new state based on a rule
  - Accept or reject the new state
  - Apply another random event
  - After enough steps, collect samples to estimate properties
- Properties are obtained from ensemble average

Molecular Dynamics Simulation

❑ Molecular Dynamics:

It is a deterministic approach for investigating material properties from atomistic simulations of time-evolving trajectories using time average

- Differential equations of motion are solved numerically to obtain the positions and velocities of atoms or particles
- It is typically applied to an isolated system containing a fixed number of atoms N in a fixed volume V
- Properties are calculated through time averaging.

Ergodic hypothesis: Ensemble average = time average

Molecular Dynamics Simulation

MD simulation

Generating trajectories

Analyzing trajectories

Initialization

Equilibration

Production

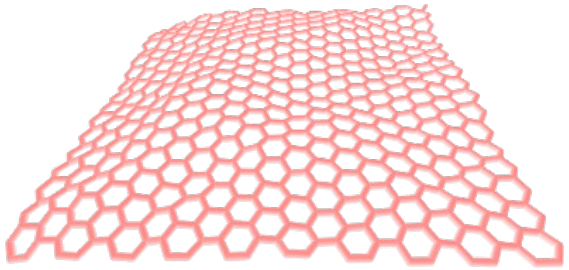
Atomic structure

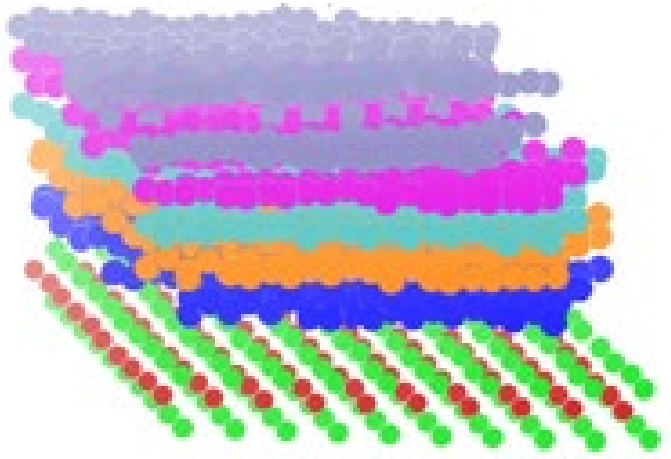
Atomic interactions

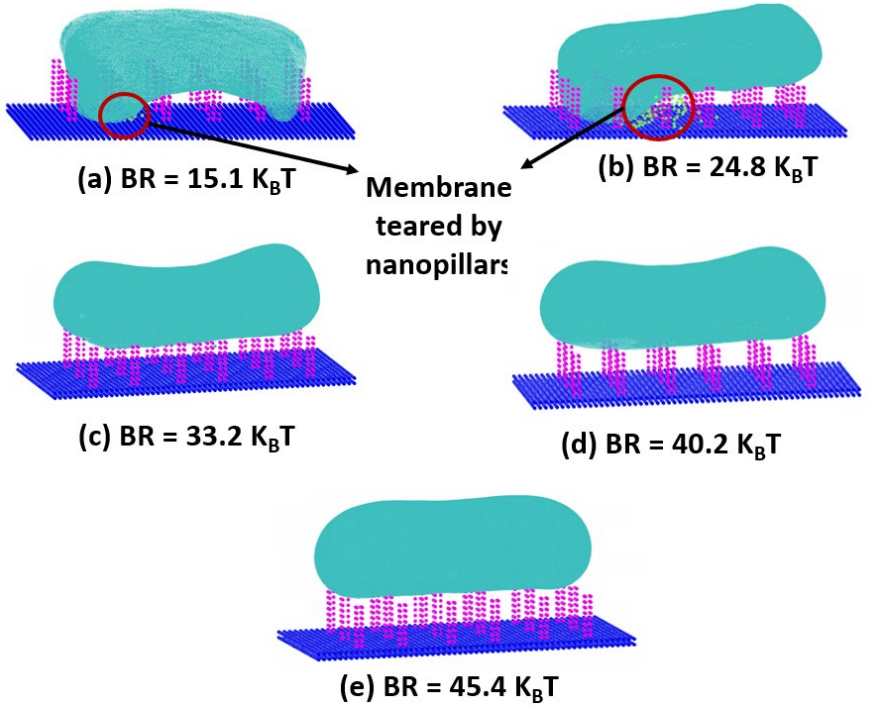
Boundary conditions

Initial state

Atomic structure







Atomic Interactions

- Bond types:
  - Metallic bonds-> Embedded atom: an atom in the electron cloud soup of the neighbor atoms
  - Ionic bonds-> Coulombic interactions: charged neigbors
  - Co-valent bonds
  - Non-covalent interactions

- Interatomic potentials:
  - Embedded Atom Model
  - Lennard-Jones
  - Bond-order potential

Equilibriation

- After the initialization, the system trajectories converge from an arbitrary initial state to the equilibrium state over a short period
  - Use finite difference algorithm to generate phase-space trajectories from initial conditions
  - Atoms move according to Newton's law:
  - Monitor certain properties that are based on phase-space trajectories
  - Scale velocity to maintain temperature

Output from MD simulations

- Analyze trajectories for macroscopic properties: compute statistical averages from time averages

  - Static properties
    - Thermodynamic properties
    - Static structure: measure in terms of radial distribution function of neighboring atoms
  - Dynamic properties: time correlation functions
    - Viscosity, thermal conductivity, diffusivity